

# Redetermination of Dy<sub>3</sub>Ni from single-crystal X-ray data

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Dy-Ni}) = 0.003$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.052; data-to-parameter ratio = 25.3.

The classification of the title compound, tridysprosium nickel, into the Fe<sub>3</sub>C (or Al<sub>3</sub>Ni) structure type has been deduced from powder X-ray diffraction data with lattice parameters reported in a previous study [Lemaire & Paccard (1967). *Bull. Soc. Fr. Mineral. Cristallogr.* **40**, 311–315]. The current re-investigation of Dy<sub>3</sub>Ni based on single-crystal X-ray data revealed atomic positional parameters and anisotropic displacement parameters with high precision. The asymmetric unit consists of two Dy and one Ni atoms. One Dy atom has site symmetry  $m$ . (Wyckoff position 4c) and is surrounded by twelve Dy and three Ni atoms. The other Dy atom (site symmetry 1, 8d) has eleven Dy and three Ni atoms as neighbours, forming a distorted Frank–Kasper polyhedron. The coordination polyhedron of the Ni atom ( $m$ , 4c) is a tricapped trigonal prism formed by nine Dy atoms.

## Related literature

For a previous crystallographic investigation of the title compound, see: Lemaire & Paccard (1967). For the Fe<sub>3</sub>C structure, see: Hendricks (1930), and for the Al<sub>3</sub>Ni structure, see: Bradley & Taylor (1937). For the Dy–Ni phase diagram, see: Zheng & Wang (1982). For magnetic properties of Dy<sub>3</sub>Ni, see: Talik *et al.* (1996), and for magnetic properties of Dy<sub>3</sub>Co, see: Baranov *et al.* (1995). For isotypic compounds, see: Tsvyashchenko (1986); Romaka *et al.* (2011); Buschow & van der Goot (1969); Givord & Lemaire (1971). For structure refinements of other compounds in the Dy–Ni system, see: Levytskyi *et al.* (2012a,b).

## Experimental

### Crystal data

Dy <sub>3</sub> Ni	$V = 413.2$ (3) Å <sup>3</sup>
$M_r = 546.21$	$Z = 4$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
$a = 6.863$ (3) Å	$\mu = 57.86$ mm <sup>−1</sup>
$b = 9.553$ (3) Å	$T = 293$ K
$c = 6.302$ (2) Å	$0.14 \times 0.11 \times 0.10$ mm

### Data collection

Stoe IPDS II diffractometer	973 measured reflections
Absorption correction: numerical ( $X$ -RED; Stoe & Cie, 2009)	582 independent reflections
$T_{\min} = 0.007$ , $T_{\max} = 0.026$	447 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.042$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	23 parameters
$wR(F^2) = 0.052$	$\Delta\rho_{\max} = 2.82$ e Å <sup>−3</sup>
$S = 1.12$	$\Delta\rho_{\min} = -2.65$ e Å <sup>−3</sup>
582 reflections	

Data collection: *X-Area* (Stoe & Cie, 2009); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SIR2011* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2777).

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## supplementary materials

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## Redetermination of Dy<sub>3</sub>Ni from single-crystal X-ray data

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### 1. Comment

Lattice parameters for  $RE_3Ni$  compounds with  $RE = Y, La, Pr, Nd, Sm, Gd-Tm$ , have been determined and their crystal structures reported to be isotypic with the  $Fe_3C$  (or  $Al_3Ni$ ) type structure which includes also  $Dy_3Ni$  (Lemaire & Paccard, 1967). According to the phase diagram of the Dy–Ni system (Zheng & Wang, 1982),  $Dy_3Ni$  is stable below 1035 K and is formed by the peritectic reaction:  $Dy + L \rightarrow Dy_3Ni$ .

Similar isotypic  $RE_3Co$  compounds were also reported (Buschow & van der Goot, 1969) for  $RE = Y, La, Pr, Nd, Sm, Gd-Er$ .  $Lu_3Co$  has been prepared by Givord & Lemaire (1971),  $Lu_3Ni$  by Romaka *et al.* (2011). Tsvyashchenko (1986) synthesized  $Yb_3Co$  and  $Yb_3Ni$  at high pressure. According to Tsvyashchenko (1986),  $Yb_3Co$  adopts the  $Fe_3C$  type structure and  $Yb_3Ni$  the  $Al_3Ni$  structure type. On the other hand, Lemaire & Paccard (1967) claimed the  $RE_3Ni$  compounds to have the same structure as the  $RE_3Co$  compounds. To clarify the confusion with the assigned structure types, we have studied literature data for the  $Fe_3C$  (Hendricks, 1930) and the  $Al_3Ni$  (Bradley & Taylor, 1937) prototype structures, concluding that  $Al_3Ni$  and  $Fe_3C$  are isotypic. In accordance with the majority in literature, we will use the  $Fe_3C$  structure type for classification as it has been reported earlier.

Recently, two binary compounds of the Dy–Ni system have been redetermined using single-crystal X-ray data (Levytskyy *et al.*, 2012*a,b*). Here we present the results of the single-crystal X-ray analysis of  $Dy_3Ni$ . Details of the crystal structure have not been investigated before, and only isotypism with the  $Fe_3C$  was reported together with lattice parameters (Lemaire & Paccard, 1967).

The structure of  $Dy_3Ni$  is characterized by formation of trigonal prisms of Dy atoms with Ni atom enclosed in the centre. A view of the crystal structure of  $Dy_3Ni$  is shown in Fig. 1. The value of the displacement parameter  $U_{22}$  for the Ni atom displays a high anisotropy in the  $b$  direction which may have an influence on some physical properties of the compound. Magnetic properties of  $Dy_3Ni$  were reported by Talik *et al.* (1996) and generally confirm this assumption which is also valid for the isotypic  $Dy_3Co$  (Baranov *et al.*, 1995).

In Fig. 2 the  $ac$  projection of the unit cell and the coordination polyhedra for all atom types in  $Dy_3Ni$  are shown. The coordination number for Dy1 (site symmetry  $.m.$ , Wyckoff site 4  $c$ ) is 15 with bonding to 12 Dy and 3 Ni atoms. The coordination number for Dy2 (site symmetry 1, Wyckoff site 8  $d$ ) is 14, resulting in a distorted Frank–Kasper polyhedron defined by 11 Dy and 3 Ni atoms. The coordination number for Ni (site symmetry  $.m.$ , Wyckoff site 4  $c$ ) is 9, resulting in a slightly distorted tricapped trigonal prism made up of 9 Dy atoms.

The analysis of interatomic distances shows a slight decrease of some Dy–Ni distances. This feature is in good agreement with the observed Ho–Co distances for previously reported  $Ho_3Co$  (Buschow & van der Goot, 1969). The explanation of this fact may be deduced from an electronic band structure calculation.

## 2. Experimental

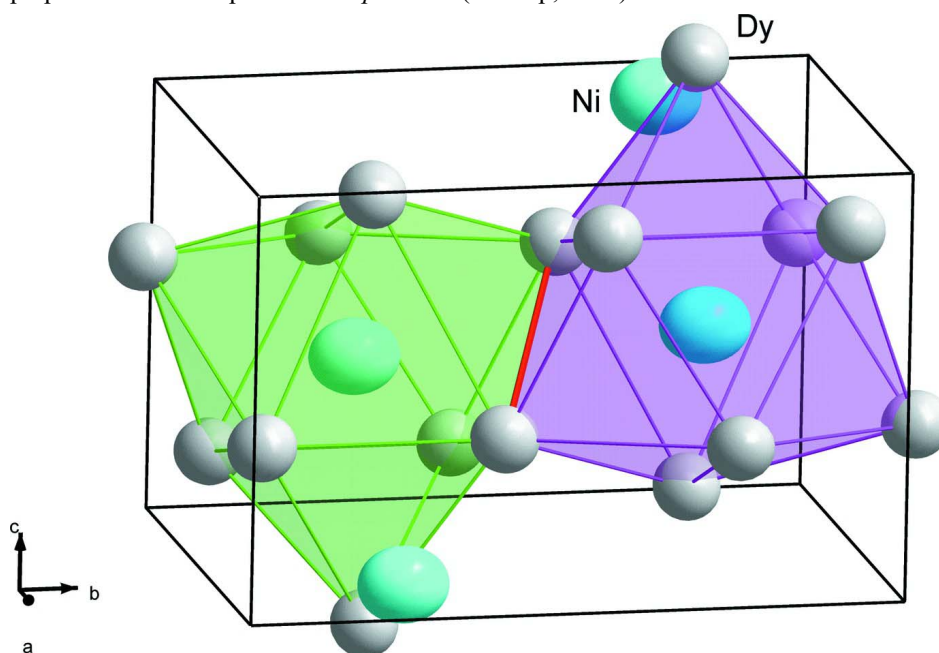
The sample was prepared from powdered commercially available pure elements: sublimed bulk pieces of dysprosium metal with a claimed purity of 99.99 at.% (Alfa Aesar, Johnson Matthey) and electrolytic nickel (99.99% pure) pieces (Aldrich). A mixture of the powders was compacted into a pellet. It was arc-melted under an argon atmosphere on a water-cooled copper hearth. The alloy button (~1 g) was turned over and remelted three times to improve homogeneity. Subsequently, the sample was annealed in an evacuated silica tube under an argon atmosphere for four weeks at 870 K. Shiny metallic gray plate-like crystals were isolated mechanically with a help of microscope by crushing the sample.

## 3. Refinement

The atomic positions found from the direct methods structure solution were in good agreement with those from the  $\text{Fe}_3\text{C}$  structure type (Hendricks, 1930) and were used as starting point for the structure refinement. The highest Fourier difference peak of  $2.82 \text{ e } \text{\AA}^{-3}$  is at  $(0.0340 \ 0.75 \ 0.1598)$  and  $1.36 \text{ \AA}$  away from the Dy2 atom. The deepest hole of  $-2.65 \text{ e } \text{\AA}^{-3}$  is at  $(0.0358 \ 0.25 \ 0.0220)$  and  $1.01 \text{ \AA}$  away from the Ni atom.

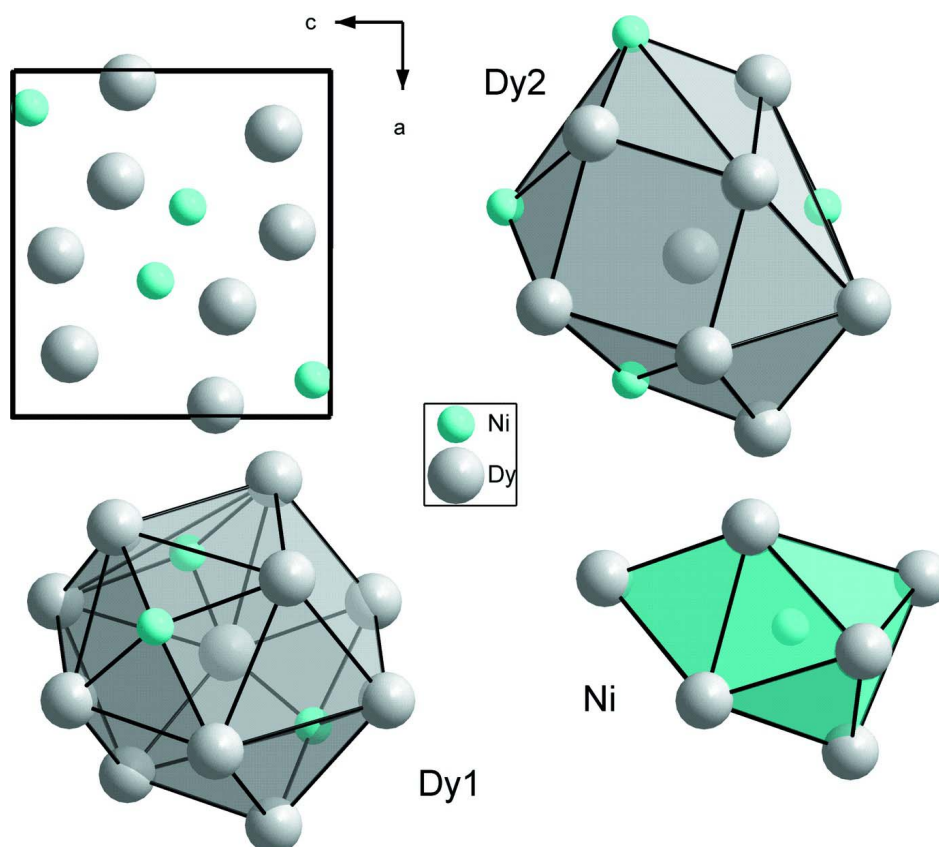
## Computing details

Data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA* (Stoe & Cie, 2009); data reduction: *X-AREA* (Stoe & Cie, 2009); program(s) used to solve structure: *SIR2011* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).



**Figure 1**

Perspective view of the crystal structure of  $\text{Dy}_3\text{Ni}$ . The unit cell and coordination trigonal prisms for Ni atoms are emphasized. The stacking edge of these prisms is marked by red colour. Atoms are represented by their anisotropic displacement ellipsoids at the 99.9% probability level.



**Figure 2**

The *ac* projection of the unit cell and coordination polyhedra for all types of atoms in the Dy<sub>3</sub>Ni structure.

### Tridysprosium nickel

#### Crystal data

Dy<sub>3</sub>Ni

$M_r = 546.21$

Orthorhombic, *Pnma*

$a = 6.863 (3) \text{ \AA}$

$b = 9.553 (3) \text{ \AA}$

$c = 6.302 (2) \text{ \AA}$

$V = 413.2 (3) \text{ \AA}^3$

$Z = 4$

$F(000) = 904$

#### Data collection

Stoe IPDS II

diffractometer

Radiation source: fine-focus sealed tube

$\omega$  scans

Absorption correction: numerical  
(*X-RED*; Stoe & Cie, 2009)

$T_{\min} = 0.007$ ,  $T_{\max} = 0.026$

973 measured reflections

$D_x = 8.781 \text{ Mg m}^{-3}$

Mo *K* $\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2575 reflections

$\theta = 3.7\text{--}29.5^\circ$

$\mu = 57.86 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, metallic gray

$0.14 \times 0.11 \times 0.10 \text{ mm}$

582 independent reflections

447 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 29.6^\circ$ ,  $\theta_{\min} = 3.9^\circ$

$h = 0 \rightarrow 9$

$k = 0 \rightarrow 12$

$l = -8 \rightarrow 8$

# Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$ 
 $wR(F^2) = 0.052$ 
 $S = 1.12$ 

582 reflections

23 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

 $w = 1/[\sigma^2(F_o^2) + (0.0141P)^2]$ 

where  $P = (F_o^2 + 2F_c^2)/3$ 
 $(\Delta/\sigma)_{\max} < 0.001$ 
 $\Delta\rho_{\max} = 2.82 \text{ e } \text{\AA}^{-3}$ 
 $\Delta\rho_{\min} = -2.65 \text{ e } \text{\AA}^{-3}$ 

Extinction correction: *SHELXL2013* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.00030 (10)

# Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

# Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Dy1	0.17975 (10)	0.06439 (6)	0.17745 (9)	0.01479 (17)
Dy2	0.03218 (14)	0.2500	0.63694 (13)	0.0147 (2)
Ni	0.3917 (4)	0.2500	0.4477 (4)	0.0197 (5)

# Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Dy1	0.0150 (3)	0.0151 (3)	0.0143 (2)	0.0001 (3)	0.0003 (3)	−0.0004 (2)
Dy2	0.0158 (5)	0.0144 (4)	0.0138 (4)	0.000	0.0014 (3)	0.000
Ni	0.0131 (12)	0.0268 (14)	0.0192 (11)	0.000	0.0003 (10)	0.000

# Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Dy1—Ni <sup>i</sup>	2.770 (2)	Dy2—Dy1 <sup>xii</sup>	3.5361 (12)
Dy1—Ni	2.856 (2)	Dy2—Dy1 <sup>vi</sup>	3.5433 (12)
Dy1—Ni <sup>ii</sup>	3.3700 (15)	Dy2—Dy1 <sup>viii</sup>	3.5944 (14)
Dy1—Dy1 <sup>iii</sup>	3.5174 (11)	Dy2—Dy1 <sup>i</sup>	3.5944 (14)
Dy1—Dy1 <sup>iv</sup>	3.5174 (11)	Dy2—Dy1 <sup>xiii</sup>	3.6047 (12)
Dy1—Dy2 <sup>v</sup>	3.5361 (12)	Dy2—Dy1 <sup>iii</sup>	3.6047 (12)
Dy1—Dy2	3.5433 (12)	Dy2—Dy2 <sup>xiv</sup>	3.7156 (15)
Dy1—Dy1 <sup>vi</sup>	3.5462 (16)	Dy2—Dy2 <sup>xi</sup>	3.7156 (15)
Dy1—Dy1 <sup>vii</sup>	3.5502 (15)	Ni—Dy1 <sup>x</sup>	2.770 (2)
Dy1—Dy1 <sup>viii</sup>	3.5512 (15)	Ni—Dy1 <sup>ix</sup>	2.770 (2)
Dy1—Dy1 <sup>ix</sup>	3.5512 (15)	Ni—Dy2 <sup>xiv</sup>	2.790 (3)
Dy1—Dy2 <sup>x</sup>	3.5944 (14)	Ni—Dy1 <sup>vi</sup>	2.856 (2)
Dy2—Ni	2.740 (3)	Ni—Dy1 <sup>xiii</sup>	3.3700 (15)
Dy2—Ni <sup>xi</sup>	2.790 (3)	Ni—Dy1 <sup>iii</sup>	3.3700 (15)
Dy2—Dy1 <sup>v</sup>	3.5361 (12)		
Ni <sup>i</sup> —Dy1—Ni	97.80 (5)	Dy1—Dy2—Dy1 <sup>vi</sup>	60.06 (3)

Ni <sup>i</sup> —Dy1—Ni <sup>ii</sup>	110.14 (3)	Ni—Dy2—Dy1 <sup>viii</sup>	111.46 (6)
Ni—Dy1—Ni <sup>ii</sup>	152.06 (4)	Ni <sup>xi</sup> —Dy2—Dy1 <sup>viii</sup>	106.54 (6)
Ni <sup>i</sup> —Dy1—Dy1 <sup>iii</sup>	132.42 (6)	Dy1 <sup>v</sup> —Dy2—Dy1 <sup>viii</sup>	59.11 (2)
Ni—Dy1—Dy1 <sup>iii</sup>	62.83 (4)	Dy1 <sup>xii</sup> —Dy2—Dy1 <sup>viii</sup>	108.94 (3)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>iii</sup>	96.49 (5)	Dy1—Dy2—Dy1 <sup>viii</sup>	59.67 (3)
Ni <sup>i</sup> —Dy1—Dy1 <sup>iv</sup>	99.46 (5)	Dy1 <sup>vi</sup> —Dy2—Dy1 <sup>viii</sup>	89.35 (3)
Ni—Dy1—Dy1 <sup>iv</sup>	127.71 (7)	Ni—Dy2—Dy1 <sup>i</sup>	111.46 (6)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>iv</sup>	48.95 (4)	Ni <sup>xi</sup> —Dy2—Dy1 <sup>i</sup>	106.54 (6)
Dy1 <sup>iii</sup> —Dy1—Dy1 <sup>iv</sup>	127.23 (4)	Dy1 <sup>v</sup> —Dy2—Dy1 <sup>i</sup>	108.94 (3)
Ni <sup>i</sup> —Dy1—Dy2 <sup>v</sup>	110.13 (6)	Dy1 <sup>xii</sup> —Dy2—Dy1 <sup>i</sup>	59.11 (2)
Ni—Dy1—Dy2 <sup>v</sup>	122.64 (5)	Dy1—Dy2—Dy1 <sup>i</sup>	89.35 (3)
Ni <sup>ii</sup> —Dy1—Dy2 <sup>v</sup>	47.57 (5)	Dy1 <sup>vi</sup> —Dy2—Dy1 <sup>i</sup>	59.67 (3)
Dy1 <sup>iii</sup> —Dy1—Dy2 <sup>v</sup>	61.27 (3)	Dy1 <sup>viii</sup> —Dy2—Dy1 <sup>i</sup>	59.12 (3)
Dy1 <sup>iv</sup> —Dy1—Dy2 <sup>v</sup>	96.43 (3)	Ni—Dy2—Dy1 <sup>xiii</sup>	62.42 (3)
Ni <sup>i</sup> —Dy1—Dy2	73.05 (5)	Ni <sup>xi</sup> —Dy2—Dy1 <sup>xiii</sup>	97.07 (4)
Ni—Dy1—Dy2	49.28 (6)	Dy1 <sup>v</sup> —Dy2—Dy1 <sup>xiii</sup>	155.48 (3)
Ni <sup>ii</sup> —Dy1—Dy2	139.07 (5)	Dy1 <sup>xii</sup> —Dy2—Dy1 <sup>xiii</sup>	59.64 (3)
Dy1 <sup>iii</sup> —Dy1—Dy2	61.40 (2)	Dy1—Dy2—Dy1 <sup>xiii</sup>	108.55 (3)
Dy1 <sup>iv</sup> —Dy1—Dy2	170.23 (3)	Dy1 <sup>vi</sup> —Dy2—Dy1 <sup>xiii</sup>	58.947 (18)
Dy2 <sup>v</sup> —Dy1—Dy2	92.13 (2)	Dy1 <sup>viii</sup> —Dy2—Dy1 <sup>xiii</sup>	144.99 (2)
Ni <sup>i</sup> —Dy1—Dy1 <sup>vi</sup>	50.21 (4)	Dy1 <sup>i</sup> —Dy2—Dy1 <sup>xiii</sup>	89.83 (3)
Ni—Dy1—Dy1 <sup>vi</sup>	51.63 (4)	Ni—Dy2—Dy1 <sup>iii</sup>	62.42 (3)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>vi</sup>	153.03 (4)	Ni <sup>xi</sup> —Dy2—Dy1 <sup>iii</sup>	97.07 (4)
Dy1 <sup>iii</sup> —Dy1—Dy1 <sup>vi</sup>	110.47 (2)	Dy1 <sup>v</sup> —Dy2—Dy1 <sup>iii</sup>	59.64 (3)
Dy1 <sup>iv</sup> —Dy1—Dy1 <sup>vi</sup>	110.47 (2)	Dy1 <sup>xii</sup> —Dy2—Dy1 <sup>iii</sup>	155.48 (3)
Dy2 <sup>v</sup> —Dy1—Dy1 <sup>vi</sup>	148.141 (19)	Dy1—Dy2—Dy1 <sup>iii</sup>	58.947 (18)
Dy2—Dy1—Dy1 <sup>vi</sup>	59.972 (15)	Dy1 <sup>vi</sup> —Dy2—Dy1 <sup>iii</sup>	108.55 (3)
Ni <sup>i</sup> —Dy1—Dy1 <sup>vii</sup>	63.03 (5)	Dy1 <sup>viii</sup> —Dy2—Dy1 <sup>iii</sup>	89.83 (3)
Ni—Dy1—Dy1 <sup>vii</sup>	160.83 (5)	Dy1 <sup>i</sup> —Dy2—Dy1 <sup>iii</sup>	144.99 (2)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>vii</sup>	47.11 (5)	Dy1 <sup>xiii</sup> —Dy2—Dy1 <sup>iii</sup>	112.85 (4)
Dy1 <sup>iii</sup> —Dy1—Dy1 <sup>vii</sup>	129.32 (4)	Ni—Dy2—Dy2 <sup>xiv</sup>	48.35 (6)
Dy1 <sup>iv</sup> —Dy1—Dy1 <sup>vii</sup>	60.32 (3)	Ni <sup>xi</sup> —Dy2—Dy2 <sup>xiv</sup>	87.67 (7)
Dy2 <sup>v</sup> —Dy1—Dy1 <sup>vii</sup>	68.17 (3)	Dy1 <sup>v</sup> —Dy2—Dy2 <sup>xiv</sup>	104.66 (3)
Dy2—Dy1—Dy1 <sup>vii</sup>	119.32 (4)	Dy1 <sup>xii</sup> —Dy2—Dy2 <sup>xiv</sup>	104.66 (3)
Dy1 <sup>vi</sup> —Dy1—Dy1 <sup>vii</sup>	110.28 (2)	Dy1—Dy2—Dy2 <sup>xiv</sup>	92.83 (3)
Ni <sup>i</sup> —Dy1—Dy1 <sup>viii</sup>	51.95 (5)	Dy1 <sup>vi</sup> —Dy2—Dy2 <sup>xiv</sup>	92.83 (3)
Ni—Dy1—Dy1 <sup>viii</sup>	109.78 (6)	Dy1 <sup>viii</sup> —Dy2—Dy2 <sup>xiv</sup>	146.39 (2)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>viii</sup>	88.29 (5)	Dy1 <sup>i</sup> —Dy2—Dy2 <sup>xiv</sup>	146.39 (2)
Dy1 <sup>iii</sup> —Dy1—Dy1 <sup>viii</sup>	91.96 (3)	Dy1 <sup>xiii</sup> —Dy2—Dy2 <sup>xiv</sup>	57.75 (2)
Dy1 <sup>iv</sup> —Dy1—Dy1 <sup>viii</sup>	119.71 (3)	Dy1 <sup>iii</sup> —Dy2—Dy2 <sup>xiv</sup>	57.75 (2)
Dy2 <sup>v</sup> —Dy1—Dy1 <sup>viii</sup>	61.14 (2)	Ni—Dy2—Dy2 <sup>xi</sup>	176.75 (7)
Dy2—Dy1—Dy1 <sup>viii</sup>	60.88 (2)	Ni <sup>xi</sup> —Dy2—Dy2 <sup>xi</sup>	47.22 (6)
Dy1 <sup>vi</sup> —Dy1—Dy1 <sup>viii</sup>	90.0	Dy1 <sup>v</sup> —Dy2—Dy2 <sup>xi</sup>	59.55 (2)
Dy1 <sup>vii</sup> —Dy1—Dy1 <sup>viii</sup>	59.38 (3)	Dy1 <sup>xii</sup> —Dy2—Dy2 <sup>xi</sup>	59.55 (2)
Ni <sup>i</sup> —Dy1—Dy1 <sup>ix</sup>	139.72 (4)	Dy1—Dy2—Dy2 <sup>xi</sup>	125.27 (3)
Ni—Dy1—Dy1 <sup>ix</sup>	49.80 (5)	Dy1 <sup>vi</sup> —Dy2—Dy2 <sup>xi</sup>	125.27 (3)
Ni <sup>ii</sup> —Dy1—Dy1 <sup>ix</sup>	104.55 (5)	Dy1 <sup>viii</sup> —Dy2—Dy2 <sup>xi</sup>	65.79 (3)
Dy1 <sup>iii</sup> —Dy1—Dy1 <sup>ix</sup>	60.29 (3)	Dy1 <sup>i</sup> —Dy2—Dy2 <sup>xi</sup>	65.79 (3)
Dy1 <sup>iv</sup> —Dy1—Dy1 <sup>ix</sup>	88.04 (3)	Dy1 <sup>xiii</sup> —Dy2—Dy2 <sup>xi</sup>	118.64 (2)

Dy2 <sup>v</sup> —Dy1—Dy1 <sup>ix</sup>	108.20 (2)	Dy1 <sup>iii</sup> —Dy2—Dy2 <sup>xi</sup>	118.64 (2)
Dy2—Dy1—Dy1 <sup>ix</sup>	93.77 (3)	Dy2 <sup>xiv</sup> —Dy2—Dy2 <sup>xi</sup>	134.90 (5)
Dy1 <sup>vi</sup> —Dy1—Dy1 <sup>ix</sup>	90.0	Dy2—Ni—Dy1 <sup>x</sup>	140.04 (4)
Dy1 <sup>vii</sup> —Dy1—Dy1 <sup>ix</sup>	146.49 (3)	Dy2—Ni—Dy1 <sup>ix</sup>	140.04 (4)
Dy1 <sup>viii</sup> —Dy1—Dy1 <sup>ix</sup>	150.16 (4)	Dy1 <sup>x</sup> —Ni—Dy1 <sup>ix</sup>	79.59 (8)
Ni <sup>i</sup> —Dy1—Dy2 <sup>x</sup>	90.43 (6)	Dy2—Ni—Dy2 <sup>xiv</sup>	84.43 (7)
Ni—Dy1—Dy2 <sup>x</sup>	71.33 (6)	Dy1 <sup>x</sup> —Ni—Dy2 <sup>xiv</sup>	91.17 (8)
Ni <sup>ii</sup> —Dy1—Dy2 <sup>x</sup>	107.50 (5)	Dy1 <sup>ix</sup> —Ni—Dy2 <sup>xiv</sup>	91.17 (8)
Dy1 <sup>iii</sup> —Dy1—Dy2 <sup>x</sup>	118.81 (4)	Dy2—Ni—Dy1	78.53 (7)
Dy1 <sup>iv</sup> —Dy1—Dy2 <sup>x</sup>	59.62 (2)	Dy1 <sup>x</sup> —Ni—Dy1	126.22 (9)
Dy2 <sup>v</sup> —Dy1—Dy2 <sup>x</sup>	151.42 (2)	Dy1 <sup>ix</sup> —Ni—Dy1	78.25 (5)
Dy2—Dy1—Dy2 <sup>x</sup>	113.33 (3)	Dy2 <sup>xiv</sup> —Ni—Dy1	137.35 (5)
Dy1 <sup>vi</sup> —Dy1—Dy2 <sup>x</sup>	60.442 (16)	Dy2—Ni—Dy1 <sup>vi</sup>	78.53 (7)
Dy1 <sup>vii</sup> —Dy1—Dy2 <sup>x</sup>	106.94 (4)	Dy1 <sup>x</sup> —Ni—Dy1 <sup>vi</sup>	78.25 (5)
Dy1 <sup>viii</sup> —Dy1—Dy2 <sup>x</sup>	142.39 (2)	Dy1 <sup>ix</sup> —Ni—Dy1 <sup>vi</sup>	126.22 (9)
Dy1 <sup>ix</sup> —Dy1—Dy2 <sup>x</sup>	59.45 (3)	Dy2 <sup>xiv</sup> —Ni—Dy1 <sup>vi</sup>	137.35 (5)
Ni—Dy2—Ni3 <sup>xi</sup>	136.02 (9)	Dy1—Ni—Dy1 <sup>vi</sup>	76.74 (7)
Ni—Dy2—Dy1 <sup>v</sup>	120.95 (2)	Dy2—Ni—Dy1 <sup>xiii</sup>	71.46 (5)
Ni <sup>xi</sup> —Dy2—Dy1 <sup>v</sup>	63.09 (3)	Dy1 <sup>x</sup> —Ni—Dy1 <sup>xiii</sup>	69.86 (3)
Ni—Dy2—Dy1 <sup>xii</sup>	120.95 (2)	Dy1 <sup>ix</sup> —Ni—Dy1 <sup>xiii</sup>	142.80 (9)
Ni <sup>xi</sup> —Dy2—Dy1 <sup>xii</sup>	63.09 (3)	Dy2 <sup>xiv</sup> —Ni—Dy1 <sup>xiii</sup>	69.34 (4)
Dy1 <sup>v</sup> —Dy2—Dy1 <sup>xii</sup>	116.28 (4)	Dy1—Ni—Dy1 <sup>xiii</sup>	137.33 (9)
Ni—Dy2—Dy1	52.19 (4)	Dy1 <sup>vi</sup> —Ni—Dy1 <sup>xiii</sup>	68.22 (3)
Ni <sup>xi</sup> —Dy2—Dy1	149.959 (16)	Dy2—Ni—Dy1 <sup>iii</sup>	71.46 (5)
Dy1 <sup>v</sup> —Dy2—Dy1	87.87 (3)	Dy1 <sup>x</sup> —Ni—Dy1 <sup>iii</sup>	142.80 (9)
Dy1 <sup>xii</sup> —Dy2—Dy1	144.38 (2)	Dy1 <sup>ix</sup> —Ni—Dy1 <sup>iii</sup>	69.86 (3)
Ni—Dy2—Dy1 <sup>vi</sup>	52.19 (4)	Dy2 <sup>xiv</sup> —Ni—Dy1 <sup>iii</sup>	69.34 (4)
Ni <sup>xi</sup> —Dy2—Dy1 <sup>vi</sup>	149.959 (16)	Dy1—Ni—Dy1 <sup>iii</sup>	68.22 (3)
Dy1 <sup>v</sup> —Dy2—Dy1 <sup>vi</sup>	144.38 (2)	Dy1 <sup>vi</sup> —Ni—Dy1 <sup>iii</sup>	137.33 (9)
Dy1 <sup>xii</sup> —Dy2—Dy1 <sup>vi</sup>	87.87 (2)	Dy1 <sup>xiii</sup> —Ni—Dy1 <sup>iii</sup>	126.05 (8)

Symmetry codes: (i)  $x-1/2, -y+1/2, -z+1/2$ ; (ii)  $-x+1/2, y-1/2, z-1/2$ ; (iii)  $-x+1/2, -y, z+1/2$ ; (iv)  $-x+1/2, -y, z-1/2$ ; (v)  $-x, -y, -z+1$ ; (vi)  $x, -y+1/2, z$ ; (vii)  $-x, -y, -z$ ; (viii)  $x-1/2, y, -z+1/2$ ; (ix)  $x+1/2, y, -z+1/2$ ; (x)  $x+1/2, -y+1/2, -z+1/2$ ; (xi)  $x-1/2, -y+1/2, -z+3/2$ ; (xii)  $-x, y+1/2, -z+1$ ; (xiii)  $-x+1/2, y+1/2, z+1/2$ ; (xiv)  $x+1/2, -y+1/2, -z+3/2$ .